

Structure of NO Molecule on MgO (100) Surface

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Beamline(s): X7B

Introduction: Studies of the adsorption of nitric oxide (NO) on the MgO (100) surface is the first in a series of investigations involving nitrogen oxides with metal oxide surfaces and is part of our ongoing studies of surface mediated chemical reactions. Our main objective is to enhance our understanding of gas-surface interactions and to apply this knowledge to the development of materials aimed at reducing atmospheric pollutants.

Methods and Materials: A combined thermodynamic and structural study of NO on MgO (100) was undertaken at the X7B beam line using a computer controlled gas adsorption isotherm apparatus. In a separate set of laboratory based experiments isotherms were recorded below the triple point (109.51K). These studies show the formation of at least two distinct layers of NO in the temperature range above 85K. From these isotherm measurements we find that each NO molecule occupies an area of 10.3\AA^2 in the monolayer phase. The isosteric heat of adsorption was determined to be 3.4 ± 0.4 kcal/mole near layer completion.

Results: Synchrotron x-ray diffraction (XRD) data were recorded in transmission using a MAR345 image plate based detector system at wavelength 0.9374\AA from a monolayer film of NO on MgO for a series of different temperatures (beam size 0.5mm and a sample-to-detector distance of 372mm). Difference spectra obtained by subtracting the diffraction data before the NO gas was admitted into the cell from x-ray data collected after the NO film was adsorbed is presented in **Figure 1**. These data which peak near 2.1\AA^{-1} in Q exhibits a “sawtooth” shaped pattern typical of a powder averaged 2D lattice. Linefits to these data suggest that NO forms a 1×1 commensurate solid structure on the MgO (100) surface (as shown in **Figure 2**). The disappearance of the diffraction profile as the temperature is increased indicates that the NO film disorders near 250 K.

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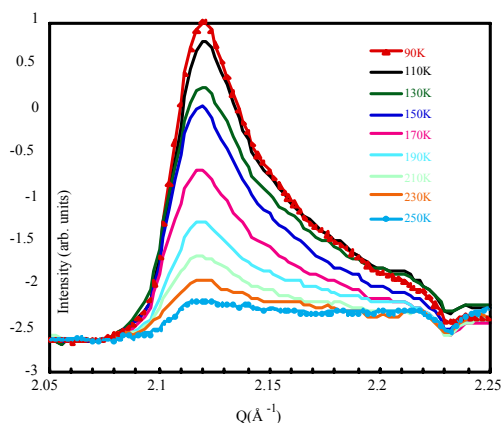


Figure 1. XRD plot of NO film on MgO (100) surface.

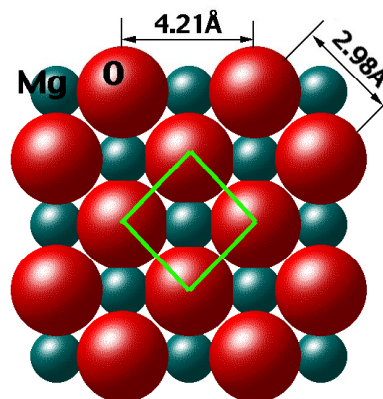


Figure 2. Schematic view of 1×1 NO molecule on Mg O (100) surface.